

Bounds on variation of the spectrum and spectral subspaces of a few-body Hamiltonian

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Abstract

We overview the recent results on the shift of the spectrum and norm bounds for variation of spectral subspaces of a Hermitian operator under an additive Hermitian perturbation. Along with the known results, we present a new subspace variation bound for the generic off-diagonal subspace perturbation problem. We also demonstrate how some of the abstract results may work for few-body Hamiltonians.

Keywords: *Few-body problem; subspace perturbation problem; variation of spectral subspace*

1 Introduction

In this short survey article we consider the problem of variation of the spectral subspace of a Hermitian operator under an additive bounded Hermitian perturbation. It is assumed that the spectral subspace is associated with an isolated spectral subset and one is only concerned with the geometric approach originating in the papers by Davis [1,2] and Davis and Kahan [3]. In this approach, a bound on the variation of a spectral subspace usually involves just two quantities: the distance between the relevant spectral subsets and a norm of the perturbation operator. We discuss only the a priori bounds, that is, the estimates that involve the distance between complementary disjoint spectral subsets of the unperturbed operator (and none of the perturbed spectral sets is involved). In the case where the perturbation is off-diagonal, we also recall the bounds on the shift of the spectrum.

The paper is organized as follows. In Section 2 we collect the results that hold for Hermitian operators of any origin. Along with the older results we present a new bound in the general off-diagonal subspace perturbation problem that was not published before. In Section 3 we reproduce several examples that illustrate the meaning of the abstract results in the context of few-body bound-state problems.

In this paper we only use the usual operator norm. For convenience of the reader, we recall that if V is a bounded linear operator on a Hilbert space \mathfrak{H} then its norm may be computed by using the formula

$$\|V\| = \sup_{f \in \mathfrak{H}, \|f\|=1} \|V|f\rangle\|$$

where \sup denotes the least upper bound. Thus, one has $\|V|f\rangle\| \leq \|V\| \|f\|$ for any $|f\rangle \in \mathfrak{H}$. If V is a Hermitian operator with $\min(\text{spec}(V)) = m_V$ and $\max(\text{spec}(V)) = M_V$ where $\text{spec}(V)$ denotes the spectrum of V , then $\|V\| = \max\{|m_V|, |M_V|\}$. In particular, if V is separable of rank one, i.e. if $V = \lambda|\phi\rangle\langle\phi|$ with $|\phi\rangle \in \mathfrak{H}$, $\|\phi\| = 1$, and $\lambda \in \mathbb{R}$, then $\|V\| = |\lambda|$. Another simple but important example is related to

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the case where $\mathfrak{H} = L_2(\mathbb{R}^n)$, $n \in \mathbb{N}$, and V is a bounded local potential, that is, $\langle x|V|f \rangle = V(x)f(x)$ for any $|f \rangle \in L_2(\mathbb{R}^n)$, with $V(\cdot)$ a bounded function from \mathbb{R}^n to \mathbb{C} . In this case $\|V\| = \sup_{x \in \mathbb{R}^n} |V(x)|$.

2 Abstract results

Let A be a Hermitian (or, equivalently, self-adjoint) operator on a separable Hilbert space \mathfrak{H} . It is well known that if V is a bounded Hermitian perturbation of A then the spectrum of the perturbed operator $H = A + V$ lies in the closed $\|V\|$ -neighborhood $\mathcal{O}_{\|V\|}(\text{spec}(A))$ of the spectrum of A (see, e.g., [4]). Hence, if a subset σ of the spectrum of A is isolated from the remainder $\Sigma = \text{spec}(A) \setminus \sigma$, then the spectrum of H also consists of two disjoint components,

$$\omega = \text{spec}(H) \cap \mathcal{O}_{\|V\|}(\sigma) \text{ and } \Omega = \text{spec}(H) \cap \mathcal{O}_{\|V\|}(\Sigma), \quad (1)$$

provided that

$$\|V\| < \frac{1}{2}d, \quad (2)$$

where

$$d := \text{dist}(\sigma, \Sigma) > 0. \quad (3)$$

Under condition (2), the separated spectral components ω and Ω of the perturbed operator H may be viewed as the result of the perturbation of the respective disjoint spectral subsets σ and Σ of the initial operator A .

Let P and Q be the spectral projections of the operators A and H associated with the respective spectral sets σ and ω , that is, $P := E_A(\sigma)$ and $Q := E_H(\omega)$. The relative position of the perturbed spectral subspace $\mathfrak{Q} := \text{Ran}(Q)$ with respect to the unperturbed one, $\mathfrak{P} := \text{Ran}(P)$, may be studied in terms of the difference $P - Q$ and, in fact, the case where $\|P - Q\| < 1$ is of particular interest. In this case the spectral projections P and Q are unitarily equivalent and the transformation from the subspace \mathfrak{P} to the subspace \mathfrak{Q} may be viewed as the direct rotation (see, e.g. [3, Sections 3 and 4]). Furthermore, one can use the quantity

$$\theta(\mathfrak{P}, \mathfrak{Q}) = \arcsin(\|P - Q\|),$$

as a measure of this rotation. This quantity is called the maximal angle between the subspaces \mathfrak{P} and \mathfrak{Q} . For a short but concise discussion of the concept of maximal angle we refer to [5, Section 2]; see also [3, 6–8]. If

$$\theta(\mathfrak{P}, \mathfrak{Q}) < \frac{\pi}{2} \quad (4)$$

and, thus, $\|P - Q\| < 1$, the subspaces \mathfrak{P} and \mathfrak{Q} are said to be in the acute-angle case.

Among the problems being solved in the subspace perturbation theory, the first and rather basic problem is to find an answer to the question on whether the requirement (2) is sufficient for the unperturbed and perturbed spectral subspaces \mathfrak{P} and \mathfrak{Q} to be in the acute-angle case, or, in order to ensure (4), one has to impose a stronger condition $\|V\| < c d$ with some $c < \frac{1}{2}$. More precisely, the question is as follows.

- (i) What is the largest possible constant c_* in the inequality

$$\|V\| < c_* d \quad (5)$$

securing the subspace variation bound (4)?

Another, practically important question is about the largest possible size of the subspace variation:

(ii) What function $M : [0, c_*) \mapsto [0, \frac{\pi}{2})$ is best possible in the bound

$$\theta(\mathfrak{P}, \mathfrak{Q}) \leq M\left(\frac{\|V\|}{d}\right) \quad \text{for } \|V\| < c_* d? \quad (6)$$

Both the constant c_* and the function M are required to be universal in the sense that they should work simultaneously for all Hermitian operators A and V for which the conditions (2) and (3) hold.

Until now, the questions (i) and (ii) have been completely answered only for those particular mutual positions of the unperturbed spectral sets σ and Σ where one of these sets lies in a finite or infinite gap of the other one, say, σ lies in a gap of Σ . For such mutual positions,

$$c_* = \frac{1}{2} \quad \text{and} \quad M(x) = \frac{1}{2} \arcsin(2x). \quad (7)$$

This result is contained in the Davis-Kahan $\sin 2\theta$ theorem (see [3]).

In the general case where no assumptions are done on the mutual position of σ and Σ , except for condition (2), the best available answers to the questions (i) and (ii) are based on the bound

$$\theta(\mathfrak{P}, \mathfrak{Q}) \leq \frac{1}{2} \arcsin \frac{\pi \|V\|}{d} \quad \text{if } \|V\| \leq \frac{1}{\pi} d \quad (8)$$

proven in [5] and called there the generic $\sin 2\theta$ estimate. The bound (8) remains the strongest known bound for $\theta(\mathfrak{P}, \mathfrak{Q})$ whenever $\|V\| \leq \frac{4}{\pi^2 + 4} d$ (see [5, Remark 4.4]; cf. [8, Corollary 2]).

In [5], it has been shown that the bound (8) can also be used to obtain estimates of the form (6) for $\|V\| > \frac{1}{\pi} d$. To this end, one introduces the operator path $H_t = A + tV$, $t \in [0, 1]$, and chooses a set of points

$$0 = t_0 < t_1 < t_2 < \dots < t_n = 1 \quad (9)$$

in such a way that

$$\frac{(t_{j+1} - t_j) \|V\|}{\text{dist}(\omega_{t_j}, \Omega_{t_j})} \leq \frac{1}{\pi}, \quad (10)$$

where ω_t and Ω_t denote the disjoint spectral components of H_t originating from σ and Σ , respectively; $\omega_t = \text{spec}(H_t) \cap \mathcal{O}_{d/2}(\sigma)$ and $\Omega_t = \text{spec}(H_t) \cap \mathcal{O}_{d/2}(\Sigma)$. Applying the estimate (8) to the maximal angle between the spectral subspaces $\text{Ran}(\mathbf{E}_{H_{t_j}}(\omega_{t_j}))$ and $\text{Ran}(\mathbf{E}_{H_{t_{j+1}}}(\omega_{t_{j+1}}))$ of the corresponding consecutive operators H_{t_j} and $H_{t_{j+1}}$ and using, step by step, the triangle inequality for the maximal angles (see [9]; cf. [5, Lemma 2.15]) one arrives at the optimization problem

$$\arcsin(\|P - Q\|) \leq \frac{1}{2} \inf_{n, \{t_i\}_{i=0}^n} \sum_{j=0}^{n-1} \arcsin \frac{\pi(t_{j+1} - t_j) \|V\|}{\text{dist}(\omega_{t_j}, \Omega_{t_j})}, \quad (11)$$

over $n \in \mathbb{N}$ and $\{t_i\}_{i=0}^n$ chosen accordingly to (9) and (10). Taking into account that

$$\text{dist}(\omega_{t_j}, \Omega_{t_j}) \geq d - 2\|V\|t_j,$$

from (11) one then deduces the bound

$$\theta(\mathfrak{P}, \mathfrak{Q}) \leq M_{\text{gen}}\left(\frac{\|V\|}{d}\right) \quad (12)$$

with the estimating function $M_{\text{gen}}(x)$, $x \in [0, \frac{1}{2})$, given by

$$M_{\text{gen}}(x) = \frac{1}{2} \inf_{n, \{\kappa_i\}_{i=0}^n} \sum_{j=0}^{n-1} \arcsin \frac{\pi(\kappa_{j+1} - \kappa_j)}{1 - 2\kappa_j}, \quad (13)$$

where the points

$$0 = \kappa_0 < \kappa_1 < \kappa_2 < \dots < \kappa_n = x \quad (14)$$

should be such that

$$\frac{\kappa_{j+1} - \kappa_j}{1 - 2\kappa_j} \leq \frac{1}{\pi}.$$

An explicit expression for the function M_{gen} has been found by Seelmann in [10, Theorem 1]. From [10, Theorem 1] it also follows that the generic optimal constant c_* in (5) satisfies inequalities

$$c_s \leq c_* \leq \frac{1}{2},$$

where

$$c_s = \frac{1}{2} - \frac{1}{2} \left(1 - \frac{\sqrt{3}}{\pi}\right)^3 = 0.454839\dots \quad (15)$$

The earlier results from [5], [11], and [12] concerning the generic bound (6) might be of interest, too.

The questions like (i) and (ii) have been addressed as well in the case of off-diagonal perturbations. Recall that a bounded operator V is said to be off-diagonal with respect to the partition $\text{spec}(A) = \sigma \cup \Sigma$ of the spectrum of A with $\sigma \cap \Sigma = \emptyset$ if V anticommutes with the difference $P - P^\perp$ of the spectral projections $P = E_A(\sigma)$ and $P^\perp = E_A(\Sigma)$, that is, if

$$V(P - P^\perp) = -(P - P^\perp)V.$$

When considering an off-diagonal Hermitian perturbation, one should take into account that conditions ensuring the disjointness of the respective perturbed spectral components ω and Ω originating from σ and Σ are much weaker than the condition (2). In particular, if the sets σ and Σ are subordinated, say $\max(\sigma) < \min(\Sigma)$, then for any (arbitrarily large) $\|V\|$ no spectrum of $H = A + V$ enters the open interval between $\max(\sigma)$ and $\min(\Sigma)$ (see, e.g., [13, Remark 2.5.19]). In such a case the maximal angle $\theta(\mathfrak{P}, \mathfrak{Q})$ between the unperturbed and perturbed spectral subspaces \mathfrak{P} and \mathfrak{Q} admits a sharp bound of the form (6) with

$$M(x) = \frac{1}{2} \arctan(2x), \quad x \in [0, \infty). \quad (16)$$

This is the consequence of the celebrated Davis-Kahan $\tan 2\theta$ theorem [3] (also, cf. the extensions of the $\tan 2\theta$ theorem in [6, 7, 14]).

If it is known that the set σ lies in a finite gap of the set Σ then the disjointness of the perturbed spectral components ω and Ω is guaranteed by the (sharp) condition $\|V\| < \sqrt{2}d$. The same condition is optimal for the bound (4) to hold. Both these results have been established in [15]. An explicit expression for the best possible function M in the corresponding estimate (6),

$$M(x) = \arctan x, \quad x \in [0, \sqrt{2}),$$

was found in [7, 16].

As for the generic case — with no restrictions on the mutual position of the spectral components σ and Σ , the condition

$$\|V\| < \frac{\sqrt{3}}{2}d \quad (17)$$

is known to be optimal in order to ensure that the gaps between σ and Σ do not close under an off-diagonal V . Moreover, under this condition for the perturbed spectral sets ω and Ω we have the following enclosures:

$$\omega \subset \mathcal{O}_{\epsilon_V}(\sigma) \quad \text{and} \quad \Omega \subset \mathcal{O}_{\epsilon_V}(\Sigma)$$

with

$$\epsilon_V = \|V\| \tan \left(\frac{1}{2} \arctan \frac{2\|V\|}{d} \right) < \frac{d}{2} \quad (18)$$

and, hence,

$$\text{dist}(\omega, \Omega) \geq d - 2\epsilon_V > 0. \quad (19)$$

The corresponding proofs were given initially in [17, Theorem 1] for bounded A and then in [13, Proposition 2.5.22] for unbounded A . From (17) it follows that the optimal constant c_* in the condition (5) ensuring the strict inequality (4) in the generic off-diagonal case necessarily satisfies the upper bound

$$c_* \leq \frac{\sqrt{3}}{2} \quad (= 0.866025\dots). \quad (20)$$

Now we employ the approach of [5] in order to get a lower bound for the above constant c_* . To this end, we simply apply the optimization estimate (11) to the off-diagonal perturbations. Due to (19), for the disjoint spectral components ω_{t_j} and Ω_{t_j} of the operator $H_{t_j} = A + t_j V$ we have

$$\begin{aligned} \text{dist}(\omega_{t_j}, \Omega_{t_j}) &\geq d - 2t_j \|V\| \tan \left(\frac{1}{2} \arctan \frac{2t_j \|V\|}{d} \right) \\ &= 2d - \sqrt{d^2 + 4t_j^2 \|V\|^2}. \end{aligned}$$

The estimate (11) then yields

$$\theta(\mathfrak{P}, \mathfrak{Q}) \leq M_{\text{off}} \left(\frac{\|V\|}{d} \right) \quad (21)$$

with the function $M_{\text{off}}(x)$, $x \in [0, \frac{\sqrt{3}}{2})$, given by

$$M_{\text{off}}(x) = \frac{1}{2} \inf_{n, \{\varkappa_i\}_{i=0}^n} \sum_{j=0}^{n-1} \arcsin \frac{\pi(\varkappa_{j+1} - \varkappa_j)}{2 - \sqrt{1 + 4\varkappa_j^2}}, \quad (22)$$

where $\varkappa_0 = 0$, $\varkappa_n = x$, and the remaining points \varkappa_j , $j = 1, 2, \dots, n-1$, should satisfy inequalities

$$0 < \frac{\varkappa_{j+1} - \varkappa_j}{2 - \sqrt{1 + 4\varkappa_j^2}} \leq \frac{1}{\pi}.$$

We have only performed a partial numerical optimization of the r.h.s. term in (22) restricting ourselves to the case where the final function is smooth. As a result, our numerical approximation $\widetilde{M}_{\text{off}}$ for the estimating function M_{off} for sure satisfies the bound

$$\widetilde{M}_{\text{off}}(x) \geq M_{\text{off}}(x) \quad \text{for all } x \in [0, \frac{\sqrt{3}}{2}). \quad (23)$$

The numerical function $\widetilde{M}_{\text{off}}(x)$ is plotted in Fig.1 along with the two previously known estimating functions

$$M_{\text{KMM}}(x) = \arcsin \left(\min \left\{ 1, \frac{\pi x}{3 - \sqrt{1 + 4x^2}} \right\} \right), \quad x \in [0, \frac{\sqrt{3}}{2}),$$

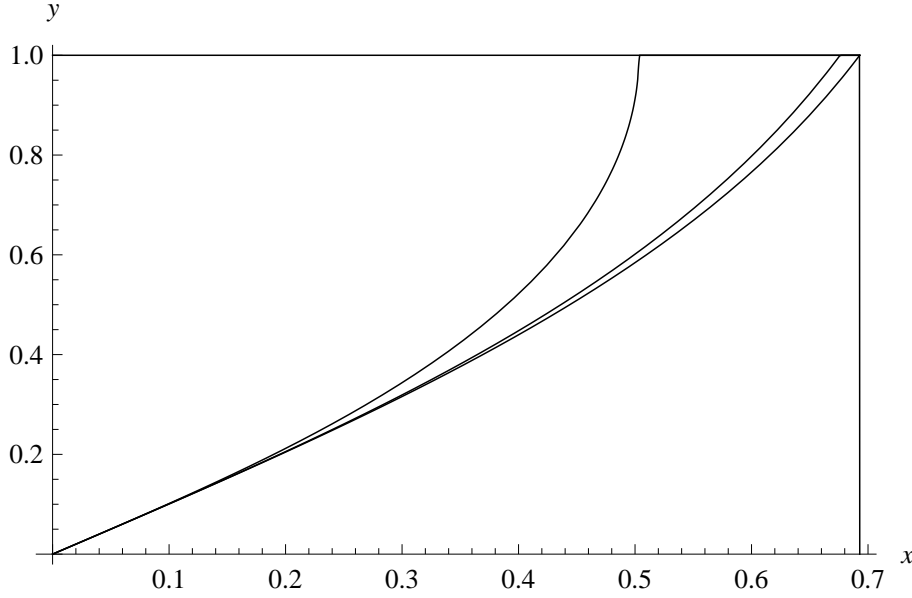


Figure 1: Graphs of the functions $\frac{2}{\pi}M_{\text{KMM}}(x)$, $\frac{2}{\pi}M_{\text{MS}}(x)$, and the numerical approximation $\frac{2}{\pi}\widetilde{M}_{\text{off}}(x)$ for $\frac{2}{\pi}M_{\text{off}}(x)$ while its value does not exceed 1. The upper curve depicts the graph of $\frac{2}{\pi}M_{\text{KMM}}(x)$, the intermediate curve is the graph of $\frac{2}{\pi}M_{\text{MS}}(x)$, and the lower curve represents the graph of $\frac{2}{\pi}\widetilde{M}_{\text{off}}(x)$.

from [17, Theorem 2] and

$$M_{\text{MS}}(x) = \arcsin \left(\min \left\{ 1, \frac{\pi}{2} \int_0^x \frac{d\tau}{2 - \sqrt{1 + 4\tau^2}} \right\} \right), \quad x \in \left[0, \frac{\sqrt{3}}{2}\right),$$

from [12, Theorem 3.3] that both serve as M in the bound (6) for the case of off-diagonal perturbations. For convenience of the reader, in the plot we divide all the three functions M_{KMM} , M_{MS} , and $\widetilde{M}_{\text{off}}$ by $\pi/2$.

For the (unique) numerical solution $x = \widetilde{c}_{\text{off}}$ of the equation $\widetilde{M}_{\text{off}}(x) = \pi/2$ within the interval $[0, \frac{\sqrt{3}}{2})$ we obtain

$$\widetilde{c}_{\text{off}} = 0.692834 \dots \quad (24)$$

Since the function $\widetilde{M}_{\text{off}}$ is monotonous and inequality (23) holds, the number $\widetilde{c}_{\text{off}}$ is an approximation to the exact solution $x = c_{\text{off}} > \widetilde{c}_{\text{off}}$ of the equation $M_{\text{off}}(x) = \pi/2$. Therefore, we arrive at the new lower bound

$$c_* > 0.692834 \quad (25)$$

for the optimal constant c_* in the condition (5) ensuring the subspace variation estimate (4) in the generic off-diagonal subspace perturbation problem. The bound (25) is stronger than the corresponding best previously published bound $c_* > 0.67598$ from [12]. Furthermore, we have inequalities

$$M_{\text{off}}(x) \leq \widetilde{M}_{\text{off}}(x) < M_{\text{MS}}(x) \quad \text{for any } x \in (0, \widetilde{c}_{\text{off}}) \quad (26)$$

which show that already the approximate estimating function $\widetilde{M}_{\text{off}}$ provides a bound of the form (6) that is stronger than the best known bound (with the function M_{MS}) from [12].

3 Applications to few-body bound-state problems

From now on, we assume that the “unperturbed” Hamiltonian A has the form $A = H_0 + V_0$ where H_0 is the kinetic energy operator of an N -particle system in the c.m. frame and the potential V_0 includes only a part of the interactions that are present in the system (say, only two-body forces). The perturbation V describes the remaining part of the interactions (say, three-body forces if $N = 3$; it may also describe the effect of external fields). We consider the case where V is a bounded operator. Of course, both A and V are assumed to be Hermitian. In order to apply the abstract results mentioned in the previous section, one only needs to know the norm of the perturbation V and a very basic stuff on the spectrum of the operator A .

Examples 3.1 and 3.2 below are borrowed from [18].

The first of the examples represents a simple illustration of the Davis-Kahan $\sin 2\theta$ and $\tan 2\theta$ theorems [3].

Example 3.1 Suppose that E_0 is the ground-state (g.s.) energy of the Hamiltonian A . Also assume that the eigenvalue E_0 is simple and let $|\psi_0\rangle$ be the g.s. wave function, i.e. $A|\psi_0\rangle = E_0|\psi_0\rangle$, $\|\psi_0\| = 1$. Set $\sigma = \{E_0\}$, $\Sigma = \text{spec}(A) \setminus \{E_0\}$ and $d = \text{dist}(\sigma, \Sigma) = \min(\Sigma) - E_0$ (we notice that the set Σ is not empty since it should contain at least the essential spectrum of A). If V is such that the condition (2) holds, then the g.s. energy E'_0 of the total Hamiltonian $H = A + V$ is again a simple eigenvalue, with a g.s. wave function $|\psi'_0\rangle$, $\|\psi'_0\| = 1$. The eigenvalue E'_0 lies in the closed $\|V\|$ -neighborhood of the g.s. energy E_0 , i.e. $|E_0 - E'_0| \leq \|V\|$. The corresponding spectral projections $P = \mathbf{E}_A(\sigma)$ and $Q = \mathbf{E}_H(\omega)$ of A and H associated with the one-point spectral sets $\sigma = \{E_0\}$ and $\omega = \{E'_0\}$ read as $P = |\psi_0\rangle\langle\psi_0|$ and $Q = |\psi'_0\rangle\langle\psi'_0|$. One verifies by inspection that

$$\arcsin(\|P - Q\|) = \arccos|\langle\psi_0|\psi'_0\rangle|.$$

Surely, this means that the maximal angle $\theta(\mathfrak{P}, \mathfrak{Q})$ between the one-dimensional spectral subspaces $\mathfrak{P} = \text{Ran}(P) = \text{span}(|\psi_0\rangle)$ and $\mathfrak{Q} = \text{Ran}(Q) = \text{span}(|\psi'_0\rangle)$ is nothing but the angle between the g.s. vectors $|\psi_0\rangle$ and $|\psi'_0\rangle$. Then the Davis-Kahan $\sin 2\theta$ theorem implies (see (6) and (7)) that

$$\arccos|\langle\psi_0|\psi'_0\rangle| \leq \frac{1}{2} \arcsin \frac{2\|V\|}{d}.$$

This bound on the rotation of the ground state means, in particular, that, under the condition (2), the angle between $|\psi_0\rangle$ and $|\psi'_0\rangle$ can never exceed 45° .

If, in addition, the perturbation V is off-diagonal with respect to the partition $\text{spec}(A) = \sigma \cup \Sigma$ then for any (arbitrarily large) $\|V\|$ no spectrum of H is present in the gap between the g.s. energy E_0 and the remaining spectrum Σ of A . Moreover, there are the following sharp universal bounds for the perturbed g.s. energy E'_0 :

$$E_0 - \epsilon_V \leq E'_0 \leq E_0,$$

(see [17, Lemma 1.1] and [13, Proposition 2.5.21]). In this case, the Davis-Kahan $\tan 2\theta$ theorem [3] implies (see (6) and (16)) that

$$\arccos|\langle\psi_0|\psi'_0\rangle| \leq \frac{1}{2} \arctan \frac{2\|V\|}{d} < \frac{\pi}{4}.$$

With a minimal change, the same consideration may be extended to the case where the initial spectral set σ consists of the $n + 1$ lowest binding energies $E_0 < E_1 < \dots < E_n$, $n \geq 1$, of A . We only underline that if V is off-diagonal than for any $\|V\|$ the perturbed spectral set ω of $H = A + V$ originating from σ will necessarily be confined in the interval $[E_0 - \epsilon_V, E_n]$ where the shift ϵ_V is given by (18); the interval $(E_n, \min(\Sigma))$ will contain no spectrum of H . Furthermore, the $\tan 2\theta$ -like

estimates for the maximal angle between the spectral subspaces $\mathfrak{P} = \text{Ran}(\mathbf{E}_A(\sigma))$ and $\mathfrak{Q} = \text{Ran}(\mathbf{E}_H(\omega))$ may be done even for some unbounded V (but, instead of d and $\|V\|$, those estimates involve quadratic forms of A and V), see [7, 14].

Along with the $\sin 2\theta$ theorem, the next example illustrates the $\tan \theta$ bound from [7, 16].

Example 3.2 Suppose that $\sigma = \{E_{n+1}, E_{n+2}, \dots, E_{n+k}\}$, $n \geq 0$, $k \geq 1$, is a set formed by the consecutive binding energies of A and $\Sigma = \text{spec}(A) \setminus \sigma = \Sigma_- \cup \Sigma_+$ where Σ_- is the increasing sequence of the energy levels E_0, E_1, \dots, E_n of A that lie lower $\min(\sigma)$; Σ_+ denotes the remainder of the spectrum of A , that is, $\Sigma_+ = \text{spec}(A) \setminus (\sigma \cup \Sigma_-)$. Under condition (3), this assumption means that the set σ lies in the finite gap $(\max(\Sigma_-), \min(\Sigma_+))$ of the set Σ . If one only assumes for V the norm bound (2) and makes no assumptions on the structure of V , then not much can be said about the location of the perturbed spectral sets ω and Ω , except for (1). However the Davis-Kahan $\sin 2\theta$ theorem [3] still well applies and, thus, one has the bound

$$\theta(\mathfrak{P}, \mathfrak{Q}) \leq \frac{1}{2} \arcsin \frac{2\|V\|}{d} < \frac{\pi}{4}.$$

Much stronger conclusions are done if V is off-diagonal with respect to the partition $\text{spec}(A) = \sigma \cup \Sigma$. In Section 2, it was already mentioned that for off-diagonal V the gap-non-closing condition is of the form $\|V\| < \sqrt{2}d$ (and even a weaker but somewhat more detailed condition $\|V\| < \sqrt{dD}$ with $D = \min(\Sigma_+) - \max(\Sigma_-)$ is admitted, see [7, 15]). In this case the lower bound for the spectrum of $H = A + V$ reads as $E_0 - \epsilon_V$ where the maximal possible energy shift ϵ_V , $\epsilon_V < d$, is given again by (18). Furthermore, the perturbed spectral set ω is confined in the interval $[E_{n+1} - \epsilon_V, E_{n+k} + \epsilon_V]$, while the open intervals $(E_n, E_{n+1} - \epsilon_V)$ and $(E_{n+k} + \epsilon_V, \min(\Sigma_+))$ contain no spectrum of H . For tighter enclosures for the perturbed spectral sets ω and Ω involving the gap length D , we refer to [13, 15, 17]. In the case under consideration, the sharp bound for the size of rotation of the spectral subspace $\mathfrak{P} = \text{Ran}(\mathbf{E}_A(\sigma))$ to the spectral subspaces $\mathfrak{Q} = \text{Ran}(\mathbf{E}_H(\omega))$ is given by the a priori $\tan \theta$ theorem (see [16, Theorem 1]; cf. [7, Theorem 2]):

$$\theta(\mathfrak{P}, \mathfrak{Q}) \leq \arctan \frac{\|V\|}{d} < \arctan \sqrt{2}.$$

If the gap length D is known and $\|V\| < \sqrt{dD}$, then a stronger but more detailed estimate for $\theta(\mathfrak{P}, \mathfrak{Q})$ is available (see [16, Theorem 4.1]).

Example 3.3 models the generic spectral disposition. Assume that the binding energies of A are numbered in the increasing order, $E_0 < E_1 < \dots < E_n < \dots$, and $\sigma = \{E_0, E_2, \dots, E_{2k}\}$ is formed of the first $k+1$, $k \geq 1$, binding energies with even numbers. Let $\Sigma = \text{spec}(A) \setminus \sigma$ and, thus, Σ contains the first k binding energies $E_1, E_3, \dots, E_{2k-1}$ with the odd numbers, as well as the remaining point spectrum and the essential spectrum of A . If $d = \text{dist}(\sigma, \Sigma) > 0$ and $\|V\| < c_s d$ with c_s given by (15), then for the maximal angle $\theta(\mathfrak{P}, \mathfrak{Q})$ between the corresponding unperturbed and perturbed spectral subspaces $\mathfrak{P} = \text{Ran}(\mathbf{E}_A(\sigma))$ and $\mathfrak{Q} = \text{Ran}(\mathbf{E}_H(\omega))$ we have the bound (12).

If, in addition, the perturbation V is off-diagonal with respect to the partition $\text{spec}(A) = \sigma \cup \Sigma$ then the disjointness of the perturbed spectral components ω and Ω is guaranteed by the weaker requirement $\|V\| < \frac{\sqrt{3}}{2}d$. In this case $\omega \subset \mathcal{O}_{\epsilon_V}(\sigma)$ and $\Omega \subset \mathcal{O}_{\epsilon_V}(\Sigma)$ where ϵ_V is given by (18). Furthermore, if $\|V\| < \tilde{c}_{\text{off}} d$ where \tilde{c}_{off} is the solution (24) of the equation $\tilde{M}_{\text{off}}(x) = \pi/2$, then one can apply the bound (22).

Examples 3.1–3.3 show how one may obtain a bound on variation of the spectral subspace prior to any real calculations for the total Hamiltonian H . In order to get such a bound, only the knowledge of the values of d and $\|V\|$ is needed. Furthermore, if V is off-diagonal, by using just these two quantities one can also provide the stronger estimates (via ϵ_V) for the binding energy shifts.

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